Chapitre 1

Introduction

Let us first define frustrated magnetism. By magnetism we mean the properties of Mott insulators (also known as magnetic insulators), systems that have a charge gap and local moments coupled by exchange interactions much smaller than the charge gap so that an accurate description can be achieved with a purely magnetic model. In this lecture, we will be dealing mostly with two models of magnetism : the *Ising* model

$$H = \sum_{(i,j)} J_{ij}\sigma_i\sigma_j, \quad \sigma_i, \sigma_j = \pm 1 \text{ or } \uparrow,\downarrow \tag{1.1}$$

and the *Heisenberg* model

$$H = \sum_{(i,j)} J_{ij}\vec{S}_i \cdot \vec{S}_j \tag{1.2}$$

where the spins $\vec{S}_i$ are unit vectors in the *classical* case, and components of a quantum spin in the *quantum* case : $[S_i^\alpha, S_i^\beta] = i\epsilon^{\alpha\beta\gamma}S_i^\gamma$, and $\vec{S}_i^2 = S(S+1)$. In both cases, i and j are sites of a periodic lattice, and J_{ij} is assumed to depend only on their relative position. In the absence of strong anisotropies originating from spin-orbit coupling, the Heisenberg model is always a good starting point. If however an on-site anisotropy forces the spins to align along a certain direction (which can be different at each site), a good effective description can be achieved by keeping only the states with projection $+S$ and $-S$ along that direction, resulting in an effective Ising model. Other situations where e.g. the spins have to be perpendicular a certain direction (XY symmetry) or where anisotropic interactions such as Dzyaloshinskii-Moriya interactions of the form $\vec{D}_{ij} \cdot \vec{S}_i \times \vec{S}_j$ are present will be discussed whenever appropriate, but they are not the main focus of these lectures.

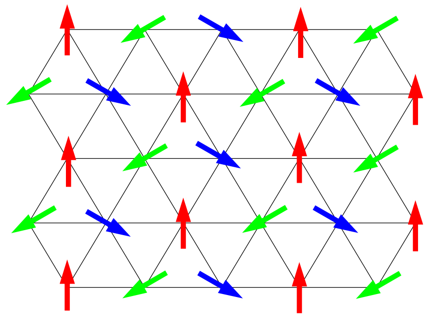

FIGURE 1.1 – Three-sbulattice order of the classical Heisenberg antiferromagnet on the triangular lattice. On each triangle, the sum of the spins must be equal to zero. Once the spins have been fixed on one triangle, the orientation of all the other spins follows from applying the rule of zero total spin on each triangle. This ground state is unique up to a global rotation of all spins.

For magnetic systems, the word frustration has been introduced in the context of spin glasses to describe the impossibility to satisfy simultaneously all exchange processes. In these lectures, we are primarily interested in disorder-free systems for which frustration is in fact better described as *geometrical frustration*, a concept that has received the following general definition : one speaks of *geometrical frustration* when a local condition is unable to lead to a simple pattern for an extended system. Typical examples are paving problems, where some figures such as triangles in 2D lead to regular, packed pavings while others such as pentagons are unable to lead to a compact, periodic structure.

In the context of magnetism, geometrical frustration can only occur if at least some exchange interactions are antiferromagnetic (i.e. favouring antiparallel alignment of spins) since, if all interactions are ferromagnetic, the configuration with all spins parallel is clearly the ground state. But even when antiferromagnetic bonds are present, geometrical frustration is not necessarily realized. Indeed, for bipartite lattices such as the square lattice (i.e. lattices that can be divided into two sublattices such that each spin of one sublattice is only coupled to spins of the other sublattice), the energy is simply minimized by by the configuration (called the Néel state) in which the spins of one sublattice are parallel to each other and antiparallel to all spins of the other sublattice. In fact, a necessary condition is to have loops of odd length. But this is by far not sufficient. Consider for instance the classical antiferromagnetic Heisenberg model on the triangular lattice :

$$E = J \sum_{\langle i,j \rangle} \vec{S}_i . \vec{S}_j, \quad J > 0 \tag{1.3}$$

where the spins $\vec{S}_i$ are vectors of length 1, and where the sum runs over all pairs of nearest neighbours. The total energy is half the sum of the energy of all elementary triangles (half to avoid double counting), and the energy of one triangle is given by

$$E_t = \vec{S}_1.\vec{S}_2 + \vec{S}_2.\vec{S}_3 + \vec{S}_3.\vec{S}_1 = \frac{J}{2}[(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 - \vec{S}_1^2 - \vec{S}_2^2 - \vec{S}_3^2]$$

or, since spins are vectors of length 1,

$$E_t = \frac{J}{2}[(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 - 3].$$

This energy is minimal if $\vec{S}_1 + \vec{S}_2 + \vec{S}_3 = 0$, which implies that the spins are coplanar at angles 120 degrees of each other (see figure). So the ground state of a triangle is unique up to a global rotation of the spins. Now, once the spins have been chosen on one triangle, the orientation of all other spins is determined by applying the triangular rule on adjacent triangles starting from the reference triangle. In other words, there is a single regular arrangement that satisfies the minimal condition on all triangles, namely a three-sublattice order in which the spins of the various sublattices are coplanar and point at 120 degrees from each other. This is a simple, regular pattern, and the Heisenberg model on the triangular lattice does not exhibit geometrical frustration according to the above definition.

In fact, in the context of classical antiferromagnets, it is usually possible to minimize the energy with a regular pattern. Geometrical frustration does not refer to the impossibility of minimizing the energy with a simple pattern. It refers to the fact that there is not a unique way to minimize the energy, but that there are other ways with less simple (often non periodic) structures to reach the ground state energy. As an example, let us consider the antiferromagnetic Ising model on the triangular lattice :

$$E = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad J > 0 \tag{1.4}$$

where $\sigma_i = \pm 1$. For Ising spins, the best one can do on a triangle is to satisfy two bonds, and all configurations with one spin in one direction and the other

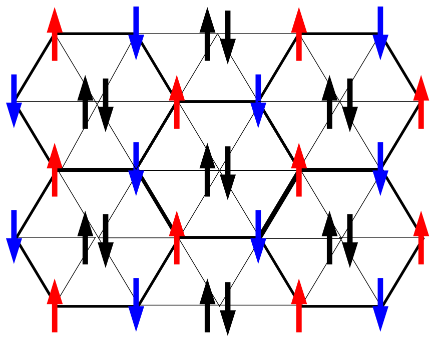

FIGURE 1.2 – Example of a family of ground states of the Ising antiferromagnet on the triangular lattice. The ground states must satisfy the rule that, on each triangle, the three spins cannot have the same orientation. Seeing the triangular lattice as a centered honeycomb lattice, one can generate an infinite number of ground states by imposing antiferromagnetic order on the honeycomb lattice. Then the local rule will be satisfied whatever the orientation of the spins sittings at the center of the hexagon, resulting in a macroscopic degeneracy and a residual entropy.

two in the other direction (i.e. all configurations which are not ferromagnetic) minimize the energy of a triangle. On an infinite system, this condition can be satisfied in an infinite number of ways. This is most easily seen by looking at the triangular lattice as a centered honeycomb lattice, i.e. a honeycomb lattice with extra spins inside the hexagons. Let us then consider configurations in which the honeycomb lattice is in antiferromagnetic state (this is possible since the honeycomb lattice is bipartite). Then the energy is minimized for any orientation of the remaining spins since each triangle contains two neighboring spins of the honeycomb lattice and thus cannot be in a ferromagnetic state. The number of such states grows with the number of sites of the triangular lattice as

$$\Omega = 2^{N/3}$$

since one third of the spins sit at the center of a hexagon, leading to a residual entropy per site

$$s = \frac{S}{N} = \frac{\ln \Omega}{N} = \frac{1}{3} \ln 2 \simeq 0.2310$$

This is actually just a lower bound. As we shall see in the next chapter,

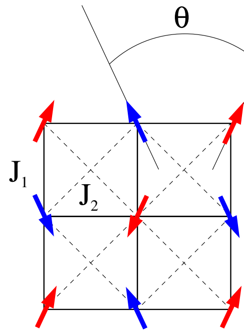

FIGURE 1.3 – Classical J_1 - J_2 antiferromagnet on the square lattice. For $J_2/J_1 > 1/2$, the energy is minimized when the two J_2 sublattices have antiferromagnetic order. The energy is then independent of J_1, resulting in an infinite degeneracy controlled by the angle θ between the sublattices.

the actual entropy can be calculated exactly, and it is significantly larger : there are many other states that minimize the energy. Note that most of these configurations are not periodic. So this is an example of geometrical frustration where a simple rule (only two parallel spins per triangle) does not lead to a simple pattern. This example is quite generic : antiferromagnetic Ising models on non-bipartite lattices exhibit geometrical frustration.

For the Heisenberg model, the example of the triangular lattice shows that this is clearly not the case. In fact, even in the presence of long-range interactions which induce odd loops, we will see that the ground state energy can be reached for a helical structure if the spins are located at the sites of a *Bravais* lattice. In general, this ground state is unique up to the choice of the pitch vector among a finite set, and it has a finite and small degeneracy. There are noticeable exceptions that we will discuss later on if the number of pitch vectors is infinite, or if helical configurations can be combined to generate new ground states. For instance, the Heisenberg model with antiferromagnetic interactions between first neigbhours (J_1) and second neighbours (J_2) has an infinite family of ground states for $J_2/J_1 > 1/2$: In that parameter range, the energy is minimized by antiferromagnetic order on each of the J_2 sublattices, and for such configurations J_1 bonds do not contribute to the energy because of the antiferromagnetic order of the four nearest neighbours of any given spin, leading to a degeneracy defined by the angle θ between the direction of the spins on the two sub-lattices. This will be discussed in more detail in the next chapter.

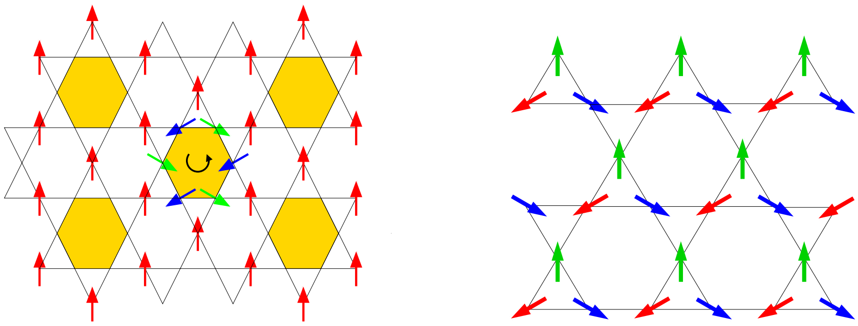

FIGURE 1.4 – Examples of families of ground states of the Heisenberg antiferromagnet on the kagome lattice. As for the triangular lattice, the energy is minimized as soon as the sum of the spins on each triangle vanishes. However, since the triangles only share corners, fixing the spins on one triangle is not sufficient to fix the orientation of the other spins. Left : Ground states where the spins between a set of non overlapping hexagons are all pallalel to a common direction. The energy will be minimized if all hexagons have the same configuration as the central one, but any configuration where the spins of each hexagon are rotated by an arbitrary angle around that of the spins sitting in between will also minimize the energy. Right : Ground state where all up (resp. down) triangles have the same order. From this state, one can generate an infinite number of ground states by rotating the spins of any straight line along the common direction of the spins adjacent to it.

However, for the Heisenberg model, geometrical frustration has far more dramatic consequences on non-Bravais lattices such as the kagome lattice in 2D or the pyrochlore lattice in 3D. In these cases, the ground state manifold has a dimension that diverges as the system size goes to infinity, and the majority of ground states are non-periodic.

1. Kagome : This is a lattice of corner sharing triangles. As for the triangular lattice the energy can be minimized independently on each triangle, but this time choosing the ground state on one triangle does not fix the spin configuration on the rest of the lattice because triangles are not sharing edges. To convince oneself that there is an infinite family of ground states, consider for instance a subset of non overlapping hexagons, and align all spins between the hexagons in the same direction. Then any of the two alternating arrangements of spins on each hexagon built out of the other two directions will

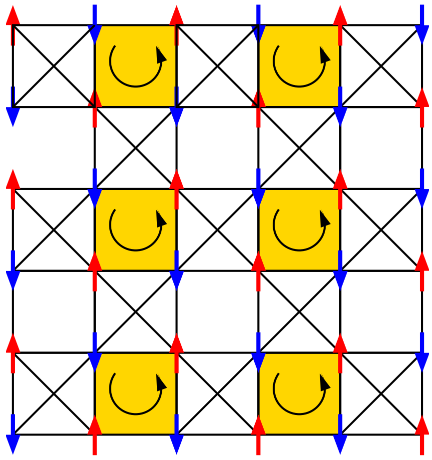

FIGURE 1.5 – Example of a family of groundstates on the checkerboard lattice. Starting from the antiferromagnetic configuration on the underlying square lattice, any configuration in which colored plaquettes have antiferromagnetic order of arbitrary direction will minimize the energy.

minimize the energy, leading to an infinite number of ground states. In fact, there are even more states because one can rotate the spins of each hexagon around the direction of the spins between the hexagons by an angle that takes a different value each hexagon, leading to non-coplanar groundstates. Alternatively, consider the configuration where all triangles are equivalent. Between two lines of spins pointing in the same direction, the spins can be rotated around the direction of those spins by an arbitrary angle.

2. Checkerboard lattice : This can be seen as a lattice of corner sharing "flattened" tetrahedra. As the triangle, the tetrahedron is a complete graph where each spin is coupled to all others, and up to a constant the energy is proportional to the square of the total spin, so that the energy is minimized as soon as, on each tetrahedron, $\sum_i \vec{S}_i = \vec{0}$. This condition is satisfied by antiferromagnetic configuration on the square lattice. However, one can again easily convince oneself that this is not the only possibility. Consider for instance a set of non overlapping empty plaquettes. Then, as for the kagome case, any antiferromagnetic state on each of these plaquettes will still satisfy the condition of zero total spin on the tetrahedra, leading again to

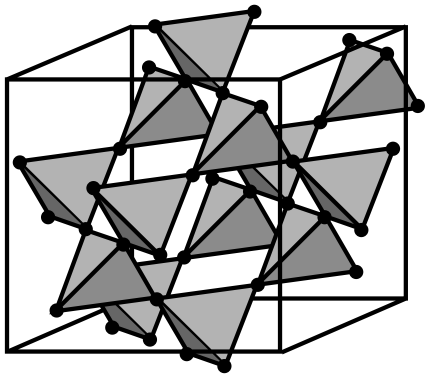

FIGURE 1.6 – Pyrochlore lattice, a lattice of corner sharing tetrahedra. As for the checkerboard lattice, the ground state of the antiferromagnetic Heisenberg model on this lattice is highly frustrated.

an infinite family of non-coplanar groundstates.

3. Pyrochlore : This is a three-dimensional lattice of corner sharing tetrahedra, and one can again generate many non-periodic ground states by adopting different antiferromagnetic configurations on a set of loops of length 6 such that each tetrahedron belongs to 2 loops.

The scope of these lectures is to investigate the physical consequences of this degeneracy. For Ising spins, this can lead to all types of zero temperature behaviors : long-range order, algebraic order, dipolar correlations or complete disorder. For Heisenberg models, fluctuations (thermal or quantum) play a major role. They can order the system by picking one ordered state out of the ground state manifold, but they can also destroy any kind of magnetic long-range order. This opens the way to new types of ground states such as spin nematics (where the order parameter is not a local spin but a more complicated object built out of several spins), valence-bond crystals (completely non-magnetic states with a broken translational symmetry), or topological spin liquids with all symmetries (spin rotation and spatial) preserved and fractional excitations.